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Shifted rectangular quadrature rule approximations to Dawson's integral $F(x)$

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Abstract

This paper investigates the relationship between some rapidly convergent series of exponential functions for computing Dawson's integral. These series are the result of approximating a certain improper integral by a shifted rectangular quadrature rule. Dawson's original method and a more recent expansion due to Rybicki are shown to be special cases of our quadrature approach. An error bound is derived to compare the accuracy of the resulting approximations. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

Dawson's integral

$$F(x)=\mathrm{e}^{-x^2}\int_0^x \mathrm{e}^{t^2}\,\mathrm{d}t \tag{1.1}$$

is encountered in physical problems, such as the calculation of absorption line profiles in astrophysics [5]. $F(x)$ is an analytic, odd function that vanishes at $x=0$ with Maclaurin series

$$F(x)=x\sum_{k=0}^{\infty}(-1)^k\frac{k!2^{2k}}{(2k+1)!}x^{2k},\quad |x|<\infty.$$

Since Dawson's early original work [3], several additional methods have been developed for the accurate numerical computation of $F(x)$. Noteworthy among these methods are: the Chebyshev series

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approximations in Hummer [6], Luke [8]; the frequently used minimax rational approximations of Cody et al. [1] and Moshier [11]. Also, see the references in [15] and the elementary exponential approximations in Lether [7].

Techniques based on approximation theory and analytical integration have also been used to express $F(x)$ as rapidly convergent series of exponential functions. For the purposes of this paper we focus attention on two of these well-known exponential series approaches.

The first series approach is based on Dawson's original 1898 work [3]. Here, we use the notation employed in Salzer [14] to conveniently summarize the basic ideas. If the known hyperbolic cosine approximation

$$e^{t^2} \approx a\pi^{-1/2}\left[1+2\sum_{n=1}^{\infty} e^{-a^2n^2}\cosh 2nat\right], \quad 0<a\leqslant 1 \tag{1.2}$$

is substituted into (1.1) we obtain Dawson's approximation

$$F(x) \approx \pi^{-1/2}e^{-x^2}\left[ax+\sum_{n=1}^{\infty} n^{-1}e^{-a^2n^2}\sinh 2nax\right], \tag{1.3}$$

where the parameter $a \in (0,1]$ remains at our disposal to control the accuracy. (Dawson chose $a=\frac{1}{2}$ in [3], since the relative error in approximation (1.2) is then less thatn $2\cdot 10^{-17}$.)

A more recent series approach is based on the sinc-approximation

$$e^{-t^2} \approx \sum_{n=-\infty}^{\infty} e^{-t_n^2}\,\mathrm{sinc}\left[\frac{\pi}{h}(t-t_n)\right], \tag{1.4}$$

where $t_n = x+nh$, $\mathrm{sinc}\, x = (\sin x)/x$ and the step size parameter $h>0$. Rybicki [13] used (1.4) in an integral representation for the complementary error function to obtain the surprising approximation [12, p. 252]

$$F(x) \approx \pi^{-1/2}\sum_{n\ \mathrm{odd}} n^{-1}e^{-(x-nh)^2}, \tag{1.5}$$

where the sum is taken over all odd positive and negative integers.

The appeal of (1.5) is due to the fact that the accuracy of the approximation increases exponentially as h decreases and moderately large values of h give very accurate approximations, due to the rapid convergence of the series. For example, the computer program in [12, p. 253] that implements a re-indexed version of (1.5) achieves an error of $2\cdot 10^{-7}$ using only 12 terms from the infinite series. This is done, in practice, using only two separate evaluations of the exponential function, by making efficient programming use of the decomposition

$$e^{-(x-nh)^2} = e^{-x^2}e^{-(nh)^2}e^{(2hx)^n}.$$

It would seem on first inspection that the approximation (1.3) and (1.5) are quite different. However, if we take $a=2h$ in (1.3) and carefully rewrite the resulting approximation we find that (1.3) becomes

$$F(x) \approx \pi^{-1/2}\left[2hxe^{-x^2}+\sum_{n\ \mathrm{even}} n^{-1}e^{-(x-nh)^2}\right], \tag{1.6}$$

where the sum is taken over all even positive and negative integers. The similarity between (1.5) and (1.6) is unexpected in view of their different underpinning approximations (1.4) and (1.2).

The purpose of this paper is to show how Rybicki's approximation (1.5) and Dawson's approximation (1.6) can both be easily obtained by approximating a certain improper integral with a primitive quadrature rule. This unifying observation is then used to derive rigorous error bounds for (1.5) and (1.6). Our error bounds for (1.5) and (1.6) turn out to be identical and show that the absolute error of Dawson's classical result (1.3), when expressed in the form (1.6), is the same as the more recent approximation (1.5).

2. A hyperbolic sine integral representation for $F(x)$

The following alternative to the usual representation (1.1) for Dawson's integral is useful for the purposes of this paper.

Lemma 1. *Dawson's function can be expressed in the form*

$$F(x)=\frac{\mathrm{e}^{-x^2}}{2\sqrt{\pi}}\int_{-\infty}^{\infty} g(t)\,\mathrm{d}t, \tag{2.1}$$

where the even function

$$g(t)=\mathrm{e}^{-t^2}t^{-1}\sinh 2xt. \tag{2.2}$$

Proof. It follows from [1, Eq. (2.6)] that $F(x)$ can be represented as the Cauchy principal value integral

$$F(x)=\frac{1}{2\sqrt{\pi}}P\int_{-\infty}^{\infty} c(t)\,\mathrm{d}t,$$

where $c(t)=t^{-1}\exp[-(t-x)^2]$. This Cauchy principal value integral can be rewritten as the ordinary improper integral [2, p. 183]

$$F(x)=\frac{1}{2\sqrt{\pi}}\int_{-\infty}^{\infty} d(t)\,\mathrm{d}t, \tag{2.3}$$

where $d(t)=[c(t)+c(-t)]/2$ is the even part of $c(t)$. A direct calculation gives $d(t)=\exp(-x^2)g(t)$ and the proof follows at once from (2.3). □

3. Shifted rectangular quadrature rule approximations to $F(x)$

If we define $g(0)=2x$, then $g(t)$ is an even, analytic function of t. In view of (2.2), $g(t)$ can be rewritten in the form

$$g(t)=\mathrm{e}^{x^2}\mathrm{e}^{-(t-x)^2}t^{-1}(1-\mathrm{e}^{-4xt})/2.$$

Consequently, the integrand in (2.1) rapidly approaches zero as $|t| \to \infty$. Under these conditions, it is well known that primitive rectangular quadrature rule over $(-\infty, \infty)$ gives surprisingly accurate results when used to approximate the integral (2.1).

The shifted rectangular quadrature rule with step h is given by

$$\int_{-\infty}^{\infty} g(t)\,\mathrm{d}t = Q(g; h, \alpha) + E(g; h, \alpha), \tag{3.1}$$

where the quadrature sum

$$Q(g; h, \alpha) = h \sum_{n=-\infty}^{\infty} g(nh + \alpha h).$$

In (3.1), the shift $\alpha \in [0, 1)$ remains at our disposal and $E(g; h, \alpha)$ denotes the quadrature error. In particular, the respective shifts $\alpha = 0$ and $\frac{1}{2}$ in (3.1) yield the familiar rectangular and midpoint quadrature rules over $(-\infty, \infty)$.

If (3.1) is applied to (2.1) we obtain the representation

$$F(x) = 2^{-1}\pi^{-1/2}\mathrm{e}^{-x^2} Q(g; h, \alpha) + R(g; h, \alpha), \tag{3.2}$$

where the error term is given by

$$R(g; h, \alpha) = 2^{-1}\pi^{-1/2}\mathrm{e}^{-x^2} E(g; h, \alpha). \tag{3.3}$$

Substituting (2.2) for g in (3.2) gives

$$F(x) = 2^{-1}\pi^{-1/2}\mathrm{e}^{-x^2} \sum_{n=-\infty}^{\infty} (n + \alpha)^{-1}\mathrm{e}^{-(n+\alpha)^2 h^2} \sinh[2(n + \alpha)hx] + R(g; h, \alpha). \tag{3.4}$$

As the following theorem shows, the error term (3.3) is negligible even for moderately large values of the step size h. For example, if $h = \frac{1}{2}$ then $|R(g; h, \alpha)| < 0.12 \cdot 10^{-17}$.

Theorem 1. *For* $\alpha \in [0, 1)$

$$|R(g; h, \alpha)| \leqslant \frac{h\mathrm{e}^{-\pi^2/h^2}}{\pi(1 - \mathrm{e}^{-2\pi^2/h^2})} \approx h\pi^{-1}\mathrm{e}^{-\pi^2/h^2}, \tag{3.5}$$

an error bound that is independent of the shift α.

Proof. Let $g(z)$ denote the analytic continuation of $g(t)$ into the complex $z = t + \mathrm{i}u$ plane. $g(z)$ is entire and therefore analytic in the infinite strip $0 \leqslant \operatorname{Im} z \leqslant s$ for any width $s > 0$. Since

$$\int_{-\infty}^{\infty} g(t)\,\mathrm{d}t = \int_{-\infty}^{\infty} g(t + \alpha h)\,\mathrm{d}t,$$

we can apply Martensen's error analysis for the basic rectangular rule [2, p. 211] to the function $2^{-1}\pi^{-1/2}\exp(-x^2)g(z + \alpha h)$ and conclude that

$$|R(g; h, \alpha)| \leqslant \frac{\pi^{-1/2}\mathrm{e}^{-x^2}}{(\mathrm{e}^{2\pi s/h} - 1)} M, \tag{3.6}$$

where

$$M=\int_{-\infty}^{\infty}|g(t+\mathrm{i}s)|\,\mathrm{d}t.$$

In view of (2.2),

$$M\leqslant s^{-1}\mathrm{e}^{s^2}\int_{-\infty}^{\infty}\mathrm{e}^{-t^2}\cosh 2xt\,\mathrm{d}t=\pi^{1/2}s^{-1}\mathrm{e}^{s^2+x^2}. \tag{3.7}$$

By (3.6) and (3.7) we have after completing the square and algebraic manipulation that

$$|R(g;h,\alpha)|\leqslant\frac{\mathrm{e}^{(s-\pi/h)^2}\mathrm{e}^{-\pi^2/h^2}}{s(1-\mathrm{e}^{-2\pi s/h})}. \tag{3.8}$$

Since the choice of the strip width s is at our disposal we select s to nearly minimize the latter bound, by choosing $s=\pi/h$. For this choice of h, (3.8) yields (3.5). □

Our interest in (3.4) stems from two basic observations that derive from re-scaling (3.4), by replacing h with $2h$. First, for $\alpha=\frac{1}{2}$ it is straightforward to show that (3.4) with step $2h$ becomes

$$F(x)=\pi^{-1/2}\mathrm{e}^{-x^2}\sum_{n\text{ odd}}n^{-1}\mathrm{e}^{-n^2h^2}\sinh 2nhx+R(g;2h,\tfrac{1}{2}),$$

or, equivalently,

$$F(x)=\pi^{-1/2}\sum_{n\text{ odd}}n^{-1}\mathrm{e}^{-(x-nh)^2}+R(g;2h,\tfrac{1}{2}),$$

which is Rybicki's approximation (1.5) with an error term $R(g;2h,\frac{1}{2})$. Second, for $\alpha=0$ (3.4) with step $2h$ becomes

$$F(x)=\pi^{-1/2}\mathrm{e}^{-x^2}\left[2hx+\sum_{n\text{ even}}n^{-1}\mathrm{e}^{-n^2h^2}\sinh 2nhx\right]+R(g;2h,0),$$

or equivalently

$$F(x)=\pi^{-1/2}\left[2hx\mathrm{e}^{-x^2}+\sum_{n\text{ even}}n^{-1}\mathrm{e}^{-(x-nh)^2}\right]+R(g;2h,0),$$

which is Dawson's approximation (1.6) with error term $R(g;2h,0)$. Consequently (1.5) and (1.6) are special cases of (3.4), whose error terms $R(g;2h,\frac{1}{2})$ and $R(g;2h,0)$ have by (3.5) a common bound

$$\frac{2h\mathrm{e}^{-\pi^2/4h^2}}{\pi(1-\mathrm{e}^{-\pi^2/2h^2})}\approx 2h\pi^{-1}\mathrm{e}^{-\pi^2/4h^2}. \tag{3.9}$$

These latter observations support the statements made in the last paragraph of Section 1 of this paper and establish the connection between the two results (1.5) and (1.6).

References

[1] W.J. Cody, K.A. Paciorek, H.C. Thacher, Chebyshev approximations of Dawson's integral, Math. Comp. 24 (1970) 171–178.
[2] P.J. Davis, P. Rabinowitz, Methods of Numerical Integration, 2nd ed., Academic Press, New York, 1984.
[3] H.G. Dawson, On the numerical value of $\int_0^h e^{x^2}\,dx$, London Math. Soc. Proc. 29 (1898) 519–522.
[4] D. Harris III, On the line absorption coefficients due to Doppler effect and damping, Astrophys. J. 108 (1948) 112–115.
[5] D.G. Hummer, Noncoherent scattering. I. The redistribution functions with Doppler broadening, Monthly Notices Roy. Astronom. Soc. 125 (1963) 21–37.
[6] D.G. Hummer, Expansion of Dawson's function in a series of Chebyshev polynomials, Math. Comp. 18 (1964) 317–319.
[7] F.G. Lether, Elementary approximations for Dawson's integral, J. Quant. Spectrosc. Radiat. Transfer 4 (1991) 343–345.
[8] Y.L. Luke, The Special Functions and Their Approximations II, Academic Press, New York, 1969.
[9] F. Matta, A. Reichel, Uniform computation of the error function and other related functions, Math. Comp. 25 (1971) 339–345.
[10] J.H. McCabe, A continued fraction expansion, with truncation error estimate, for Dawson's integral, Math. Comp. 28 (1974) 811–816.
[11] S.L. Moshier, Methods and Programs for Mathematical Functions, Ellis Horwood Limited, Chichester, 1989.
[12] W.H. Press, S.A. Teukolsky, W.T. Vettering, B.P. Flannery, Numerical Recipes in FORTRAN, The Art of Scientific Computing, 2nd ed., Cambridge University Press, Cambridge, 1992.
[13] G.B. Rybicki, Dawson's integral and the sampling theorem, Comput. Phys. 3 (1989) 85–87.
[14] H.E. Salzer, Formulas for calculating the error function of a complex variable, Math. Tables Aids Comput. 5 (1951) 67–70.
[15] C.G. van der Laan, N.M. Temme, Calculation of Special Functions: the Gamma Function, the Exponential Integrals and Error-like Functions, CWI, Amsterdam, Netherlands, 1986.